

Sodium 3-nitrobenzenesulfonate
127-68-4 | DTXSID2027048

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -1.75

Global applicability domain: Inside

Local applicability domain index: 5.87e-01

Confidence level: 3.87e-01

Nearest Neighbors from the Training Set

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4-Aminobenzenesulfonic acid

Measured: -2.16

Predicted: -2.12

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Benzenesulfonic acid, 3-amino-,
monosodium salt

Measured: -3.40

Predicted: -2.10

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4-Mesylaniline

Measured: -0.120

Predicted: -0.565

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Sodium 3-nitrobenzenesulfonate

Measured: -2.61

Predicted: -1.75

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Benzenesulfonamide, p-acetyl-
(6Cl,7Cl,8Cl)

Measured: 0.2

Predicted: 6.29e-01